Summary - Int 1, Group C, 𝚫𝚫G Version

Inbal Lorena Eshel

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# *Intermidiate 1*

## Water

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_32 + dip\_x\_1 + B5\_3\_9 | 0.658 | 0.489 | 0.325 |
| ddg ~ NPA\_32 + X.30.31. + B5\_3\_9 | 0.685 | 0.470 | 0.327 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_32 | 1.019 |
| dip\_x\_1 | 1.008 |
| B5\_3\_9 | 1.021 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.071 | 2.053 | 0.0557437 |
| NPA\_32 | -0.205 | 0.074 | -2.782 | 0.0127675 |
| dip\_x\_1 | 0.120 | 0.073 | 1.644 | 0.1186346 |
| B5\_3\_9 | -0.376 | 0.074 | -5.095 | 0.0000899 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_6 + NPA\_32 + Dist.31..36. + B5\_3\_9 | 0.751 | 0.505 | 0.294 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_6 | 1.102 |
| NPA\_32 | 2.300 |
| Dist.31..36. | 2.321 |
| B5\_3\_9 | 1.116 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.063 | 2.337 | 0.0327833 |
| NPA\_6 | -0.161 | 0.067 | -2.394 | 0.0292525 |
| NPA\_32 | -0.388 | 0.097 | -3.989 | 0.0010557 |
| Dist.31..36. | 0.214 | 0.098 | 2.190 | 0.0436963 |
| B5\_3\_9 | -0.387 | 0.068 | -5.706 | 0.0000325 |

## Methanol

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_1 + Total\_1 + B5\_3\_9 | 0.638 | 0.516 | 0.245 |
| ddg ~ dip\_y\_1 + Total\_1 + B5\_3\_9 | 0.649 | 0.514 | 0.252 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_10 + dip\_x\_1 + Dist.10..30. + B5\_3\_9 | 0.715 | 0.605 | 0.226 |
| ddg ~ NPA\_10 + dip\_z\_1 + Dist.4..10. + B5\_3\_9 | 0.702 | 0.595 | 0.242 |